

Investigation of a Tricarbide Grooved Ring Fuel Element for a Nuclear Thermal Rocket

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Deep space exploration, especially that of Mars, is on the horizon as the next big challenge for space exploration. Nuclear propulsion, through which high thrust and efficiency can be achieved, is a promising option for decreasing the cost and logistics of such a mission. Work on nuclear thermal engines goes back to the days of the NERVA program. Currently, nuclear thermal propulsion is under development again in various forms to provide a superior propulsion system for deep space exploration. The authors have been working to develop a concept nuclear thermal engine that uses a grooved ring fuel element as an alternative to the traditional hexagonal rod design. The authors are also studying the use of carbide fuels. The concept was developed in order to increase surface area and heat transfer to the propellant. The use of carbides would also raise the temperature limitations of the reactor. It is hoped that this could lead to a higher thrust to weight nuclear thermal engine. This paper describes the modeling of neutronics, heat transfer, and fluid dynamics of this alternative nuclear fuel element geometry. Fabrication experiments of grooved rings from carbide refractory metals are also presented along with material characterization and interactions with a hot hydrogen environment.

Nomenclature

K	=	Kelvin
NbC	=	Niobium Carbide
ZrC	=	Zirconium Carbide
TaC	=	Tantalum Carbide
HfC	=	Hafnium Carbide
UC	=	Uranium Carbide
VC	=	Vanadium Carbide
DCS	=	Direct Current Sintering
H_2	=	Diatomic Hydrogen
XRD	=	X-Ray Diffraction

I. Foreword

Propulsion systems that derive their power from nuclear reactions have been conceptualized for many decades. Serious efforts to develop this technology were made in both the United States and the Soviet Union. The most well known program was that of the Nuclear Engine for Rocket Vehicle Application (NERVA) that was a joint effort of the U.S. Atomic Energy Commission and NASA. Several engines were built and tested under this program

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in order to develop this technology for a manned mission to Mars. This work ran until the early 1970's.^{1,2} The reactors of the NERVA engines consisted of fuel elements formed into hexagonal rods with cylindrical flow passages through which propellant was flowed. The nuclear fission reactions heated the material in the rod and the heat was transferred to the propellant. This type of nuclear propulsion is called nuclear thermal propulsion (NTP). Later, particle bed reactors were considered in a defense project called Timberwind. This reactor geometry flowed propellant through a bed of spherical fuel "particles" to greatly increase surface area and thus heat transfer. This design showed promise for significantly improving thrust to weight ratios and specific impulse compared to the NERVA engines. It suffered; however, from nuclear thermal instabilities.²

Recently, there has been a renewed effort to develop NTP as NASA has been working seriously toward manned Mars mission planned for the 2030's. Much of the fuel fabrication and engine modelling efforts have been focused on the tungsten and graphite based fuel elements in hexagonal rod geometries. Cermet and Graphite based fuels are being studied for fuel element fabrication. This work has been moving toward the hexagonal rod geometry. The authors of this paper have been working on a center innovation fund project to investigate an alternative fuel element geometry proposed by Dr. Bill Emrich at Marshall Space Flight Center, a co-author of this paper. This concept is centered on the idea of increased surface area and heat transfer to the propellant, much as particle bed reactors do, while eliminating the thermal instabilities by creating a defined flow path. This concept is known as the grooved fuel ring element. The idea is to build a fuel element from a stack of washer like rings. Each ring has grooves cut into the surface to allow propellant, constrained by an outer structure, to flow through the grooves to the center where it can flow down and out of the reactor. This provides a large increase in surface area which is directly proportional to heat transfer. These elements would be put together to make up a reactor much in the same as traditional elements do. Figure 1 illustrates the concept.

In addition to the alternative geometry, the authors are investigating the use of mixed carbide fuels. These fuels are composed of fissile uranium carbide (UC) the fuel and additional refractory metal carbides (e.g. niobium carbide (NbC) and zirconium carbide (ZrC)) in solid solution to increase the melting temperature of UC. The Soviet Union conducted tests of carbide fuels and reached reactor temperature greater than 3000 K.¹ A combination of carbide materials has the potential to allow maximum fuel operating temperatures in the vicinity of 3500 K. This is in contrast to the lower temperature limitations of other fuel forms. The use of carbide fuels could allow the reactor to run at higher temperature and provide more thrust and specific impulse to the propulsion system.

In order to develop this alternate geometry carbide fuel element, data is needed to develop the fabrication process, understand the fuel's performance in a hot hydrogen environment and characterize material properties. This has been the primary goal of the work discussed in this paper. Past work has been studied to provide the foundation for this work.^{3,4,5,6} Additionally, modeling has been done to understand the neutronics, fluid, and heat transfer processes in such a reactor. Model results have been used to guide material selection and fabrication experiments. Processes and results to date are discussed in this document.

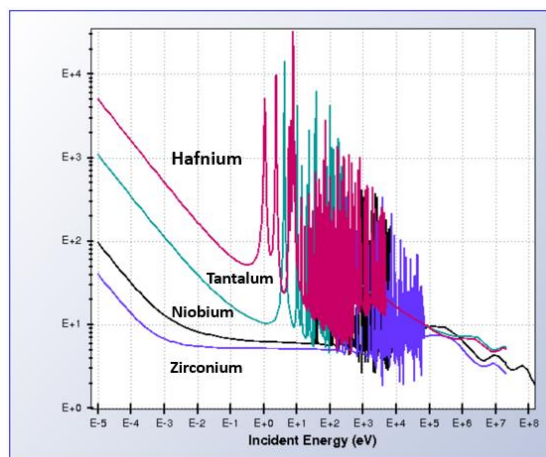


Figure 2 Cross Section of Several Refractory Metals

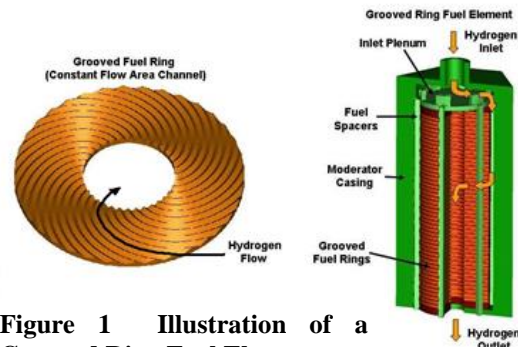


Figure 1 Illustration of a Grooved Ring Fuel Element

II. Modeling of the Neutronics for a Grooved Fuel Ring Reactor

In order to guide the selection of materials for fabrication tests, the reactor concept must be developed. The criticality and operation of the reactor is highly dependent upon material density, material selection, moderating materials, structure, etc. The model was developed with the Monte Carlo N-Particle code (MCNP). A concept layout was developed for different material combinations for a given power and thrust level. This drove the selection of materials for fabrication experiments and served as a guide for how the manufactured carbides would affect criticality and operating temperature.

A. Material Selection

The selection of carbides is a trade between high melting temperature properties and low neutron absorption cross sections. While the highest melting temperature are desired, the neutron cross section determines the quantity of uranium (UC) required for the reactor to be critical. The melting point of UC is lower than the refractory carbide compounds of interest; therefore, increasing the UC content lowers reactor temperature limits. Several refractory metals were chosen as the most promising material candidates based on past research.

Figure 2 compares the cross section of Hafnium, Tantalum, Niobium and Zirconium. One can see a significant difference between the materials. While hafnium carbide (HfC) and tantalum carbide (TaC) have the higher melting temperatures, this would be countered by the need for more UC. NbC and ZrC were chosen as the primary candidates of interest due to their lower absorption cross section. Since solid solutions containing ZrC, NbC will capture fewer neutrons, less UC is needed within the reactor. Reducing UC content will ultimately maximize the operating temperature of the fuel by allowing for the highest melting points.

B. Reactor Model

The reactor model was built using MCNP, a common nuclear physics code. The reactor model employs the grooved ring element design in a cylindrical reactor. Propellant is assumed to be hydrogen. Beryllium is used as a moderator in the core and a reflector at the boundary. The concept reactor was sized for 25,000 N of thrust with a power output of 8 kW/cm³.

Two combinations of carbides were modeled. The first configuration used a fuel mixture of UC, ZrC and NbC. The second configuration changed the mixture to UC, ZrC and TaC. The reactivity of the reactor models were analyzed to determine the amount of fuel required to operate effectively. The first carbide mixture requires a fuel to moderator ratio of 0.261 while the second carbide mixture requires a much higher fuel to moderator ratio of 2.95. Side and top views of these reactor configurations are shown in Figures 3 and 4.

Additionally, calculations were carried out to determine the impact of density on the required

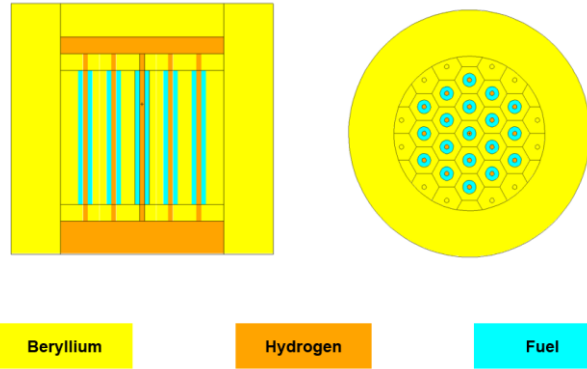


Figure 3 (U-Zr-Nb)C Fuel Reactor with fuel to moderator ratio of 0.261

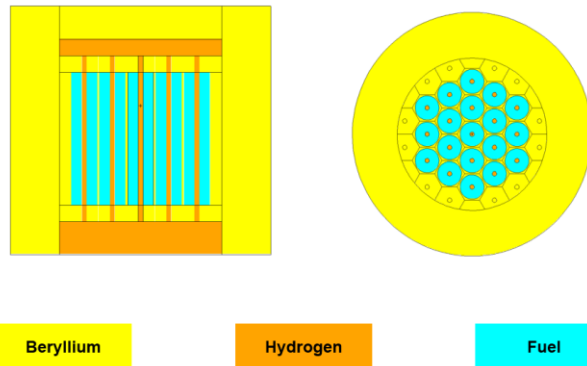


Figure 4 (U-Zr-Ta)C Fuel Reactor with fuel to moderator ratio of 2.95

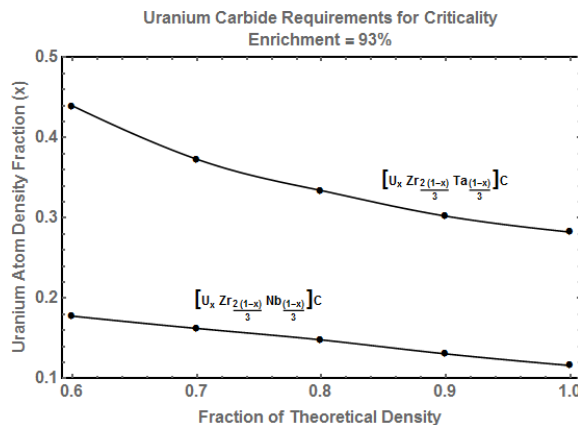


Figure 5 Uranium Carbide Requirements for Criticality

quantity of Uranium fuel. The flow paths through the grooves and center of the rings reduce the available volume of fissionable material. Also, the manufacturing process will result in small amounts of porosity. A small amount of porosity is actually required to allow room for the fission products. This is represented in terms of the percent of theoretical density. Theoretical density is 100% fuel in the ring volume. This is plotted in Figure 5. The fraction of the carbide mixture that is UC is plotted against the fraction of theoretical density. One can see that the mixture containing TaC requires much larger amounts of uranium than the NbC mixture. As the density drops

below 1, the amount of uranium needed to achieve criticality climbs. Reducing the amount of UC needed is important to raising the operational temperature of the reactor.

While the plot in Figure 5 is done for an enrichment of 95%, a better estimate of enrichment may be determined with further analysis. The less than theoretical density fuel and high neutron cross sections of the other carbides lead toward higher enrichment to counter these effects. Also, less uranium is desired to take advantage of the high melting temperatures of the other carbides. The lower uranium loading as compared with other fuel forms leads to higher enrichment. It may be, however, that if the neutron spectrum is adjusted correctly by varying the amount of moderator in the fuel element, it might be that you can still design to 20% enrichment.

III. Thermal/Fluid Model

A model of the thermal and fluid physics in a grooved ring fuel element were modeled in order to better understand the conditions needed for the propulsion system. Comsol was used to create this model. Thermal and fluid physics were coupled together in this model of a representative fuel element. Overall, the authors were looking for the pressure differential driving the flow that would be ideal for heating the propellant as well as determining the number of grooves needed to reach a reasonable mass flow rate. Conditions were adjusted based on the concept engine size of 25,000 N and 8 kW/cm³.

A. Model Description

The model attempts to represent a fuel element consisting of a stack of grooved fuel rings enclosed by a structure. The stack is limited to two rings in order to reduce computational time. This is expected to be adequate to characterize the physics of the model. The outer structure consists of a beryllium hexagon. The central stack of rings are assigned the material ZrC. As of the writing of this paper the required properties of the carbide mixture have not been measured. This will be done in order to update the model at a future date.

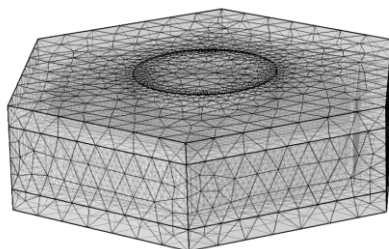


Figure 7 Mesh

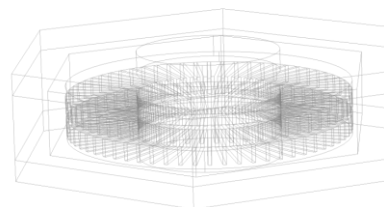


Figure 6 Wire Frame Model

The fluid is assigned as H₂ and given an inlet temperature of 500 K.

Initial temperatures are set near the inlet temperature, except for the fuel which is set to 3000 K. The pressure differential between inlet and outlet is set to 4 psi. The representative picture of the model and the corresponding mesh can be seen in the adjacent two figures.

B. Analysis of Results

Several runs of the model were performed to determine the conditions required to drive the flow through the grooves such that the propellant is heated to approximately 3000 K. The pressure differential for this geometry is 4 psi. Ideally the propellant should flow fast enough to remove enough heat that the fuel does not over heat while not moving so fast that the temperature at the outlet is too low. Figure 8 and 9 display the temperature distribution over slices of the element cut horizontally and vertically. One can see in Figure 8 the flow is heated as it passes through the grooves and exits near the max fuel temperature of 3000 K. One can examine Figure 9 to see how the central passage heats up from the flow through the grooved rings. Since this model is limited to two rings, the exit temperature is low near the axis due to the heat sink through the top of the stack to the cold propellant. A more realistic and taller stack would reach a more uniform exit temperature as more flow is heated and a longer path exists for mixing.

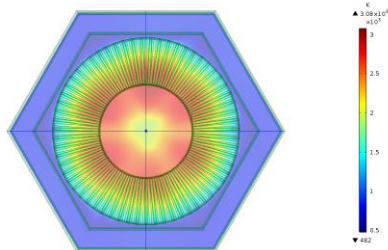


Figure 8 Top Down View of Temperature Distribution Slice

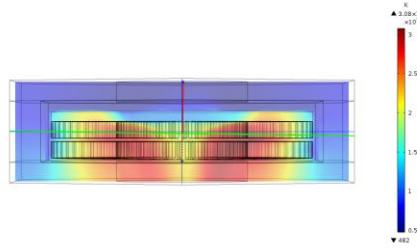


Figure 9 Side View of Temperature Distribution Slice

The velocity distribution is shown in Figures 10 and 11 as horizontal and vertical slices. Max velocities are on the order of several hundred m/s and the flow remains laminar. There is higher velocity around the corners of the inlet prior to filling the outer passage and passing through the grooves. The flow is seen to accelerate through the grooves and mix in the central passage. As mentioned before a longer more realistic stack will allow for more mixing and uniform conditions at the outlet.

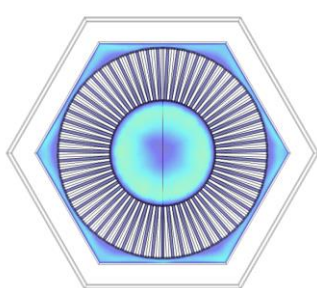


Figure 10 Top Down View of Velocity Distribution Slice

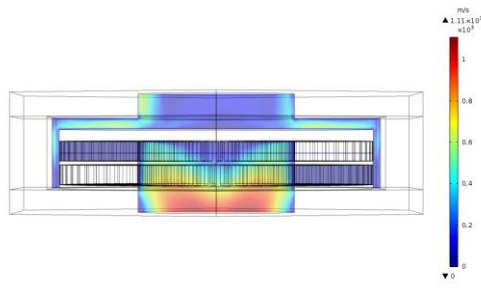


Figure 11 Side View of Velocity Distribution Slice

IV. Fabrication of a Grooved Ring Fuel Element

The optimal methods for constructing carbide fuel elements is not well understood. It is important to establish the baseline manufacture of solid solution carbides prior to proceedings with fuel element construction. To address this, the authors conducted a series of tests to determine the best method for manufacture. The authors chose to first employ direct current sintering (DCS) to create sample carbides. Hot isostatic press was determined to be a possible additional step to increase density. After sintering the sample pieces were analyzed to determine density and material distribution. Control variables were adjusted from test to test in order to work toward an optimal density and material distribution.

A. Uranium Surrogate and Material Selection

The first step in the processes of learning how to make the carbide fuels was selecting the appropriate materials. As discussed earlier, the neutron cross section has a significant impact upon the engine operation. For this reason NbC and ZrC were chosen for fabrication experiments.

A key component to the carbide fuel is of course the UC. The use of uranium; however, comes with regulatory burdens that translate into additional cost. It was practical to use a surrogate in place of uranium to reduce cost. A surrogate material with a similar crystal structure would behave in a similar manner as uranium carbide in the formation of the material, but offered significant savings and ease of use. Vanadium carbide (VC) was chosen as a surrogate since it is relatively inexpensive and forms a similar crystal structure.

The materials tested in the fabrication experiments were NbC, ZrC and VC. The quantities used were approximately 61% ZrC, 31% NbC and 8% VC by weight.

B. Powder Preparation

The carbide powders as provided by the vendors were of a nano particle size that varied within some diameter range per quality specifications. Early fabrication experiments in the DCS machine were done with raw powder as provided by the manufacturer. This created some degree of uncertainty in the results since exact particle size distribution is unknown outside of vendor specifications. This occurred due to milling equipment being out of service while being repaired. Some screening of particulate was done in later experiments to reduce the maximum particle size and limit the variability of particle diameter. At the time of writing this paper the micro mill is only recently operational, but will be used in future experiments.

C. Direct Current Sintering Experiments

The fabrication of carbide material samples were conducted using a DCS machine. This can be seen in Figure 12. Powder is loaded into a die prior to being placed in the machine. Once installed, the DCS places the sample under a pressurized inert atmosphere. It then runs a large current through the powder to raise its temperature. The machine can be controlled in several ways. Pressure, rise time, dwell time (at max temperature), and cooling rate can all be controlled. These variables were adjusted in an effort to work toward a sample with high density and good material distribution.

1. Density of Samples

High Densities were achieved earlier than anticipated. The authors were successfully able to achieve densities up to 98%. This is above the required density which is expected to be approximately 95% to accommodate fission product production.

Dwell time, cooling rate, and sintering temperature were critical variables to achieving density goals. Sintering temperatures of approximately 1600 °C were adequate to reach high densities (>95%TD). The carbides also achieved high densities at fast cooling rates. In fact the machine was turned off for a maximum cooling rate of approximately 200 C/min. The highest densities were achieved at this cooling rate. Additionally dwell times on the order of 20 minutes were adequate to give the best results. Plots of these variables can be seen in Figures 13, 14 and 15. These figures plot the percent of theoretical density as a function of sintering temperature, cooling rate, and dwell time respectively. Note that there is a good degree of variability believed to be in large part due to the variation in particle size.



Figure 12 Direct Current Sintering Machine at Marshall Space Flight Center

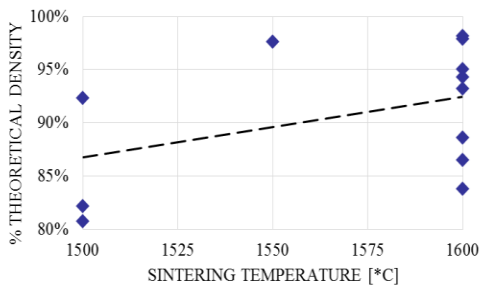


Figure 13 Percent Theoretical Density vs Sintering Temperature

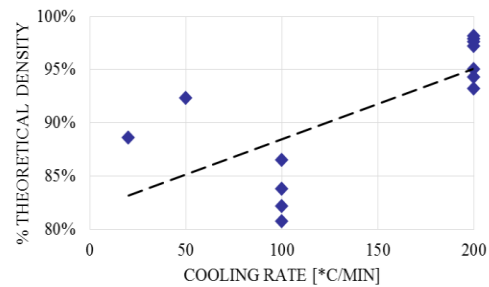


Figure 14 Percent Theoretical Density vs Cooling Rate

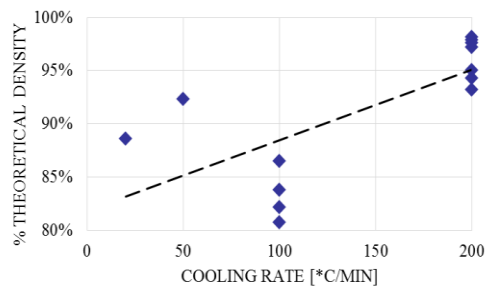


Figure 15 Percent Theoretical Density vs Dwell Time

2. Material Distribution

In order to achieve carbide fuel elements with uniform properties and best performance the distribution of the carbide elements must be as close as possible to uniform. Particle distribution of test samples were studied in addition to sample densities. Measurements were made using a scanning electron microscope and x-ray spectroscopy. The scanning electron microscope allows one to see the grain structures formed in the carbide

sample. X-ray spectroscopy is employed to identify the materials in the samples and their distribution throughout the crystal structure.

Early samples showed large grain boundaries. In these early samples the particle distribution is less than ideal. Material can be seen to be clustering together. This is believed to be in large part due to the variability in particle size with a non-optimal direct current sintering process contributing. The x-ray spectroscopy at one location of the first sample fun at 1600 degrees Celsius for 10 minutes with a 100 C/min cooling rate can be seen in Figure 16 with Table 1 showing the amount of material at the various locations.

Table 1: X-Ray Spectroscopy Analysis of Figure 16					
Material %	C	O	V	Zr	Nb
Spectrum 1	23.47		66.41	6.71	3.41
Spectrum 2	26.59	1.32	0.24	67.92	3.94
Spectrum 3	25.62	0.92	0.31	68.95	4.20
Spectrum 4	25.48	1.21	0.38	68.81	4.12
Spectrum 5	34.74	1.85		22.79	40.63
Spectrum 6	35.56	1.93	0.25	22.75	39.51
Spectrum 7	31.71	2.62	0.39	26.76	38.52

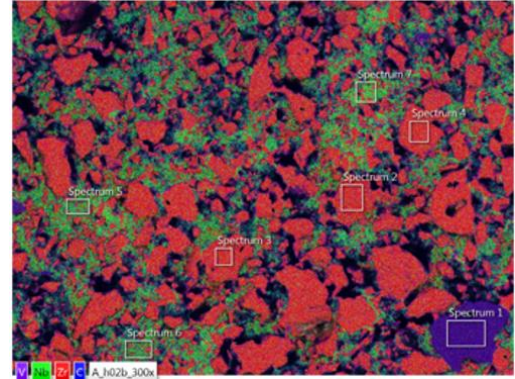


Figure 16 X-Ray Spectroscopy of First DCS Sample

After analyzing several samples the authors decided to sift the materials through a screen in order to limit the maximum particle size. This limited the particle size to 45 micron. Material screening showed improvement to the particle distribution. This can be seen in Figure 17 and Table 2.

Table 2: X-Ray Spectroscopy Analysis of Figure 17							
%	C	Ti	V	Zr	Nb	Hf	Ta
8	18.1	80.8	0	0.31			
9	18.24	1.15	78.26	0.36	0.99		
10	18.56	0.49	78.29	0.65	1.32		
11	18.94		2.1	31.08	29.87		15.91
12	16.06		3.04	25.52	33.76	21.61	
13	18.77		0.19	77.83	3.21		
14	17.67		0.44	73.07	8.81		
15	19.32		1.69	47.06	30.15		

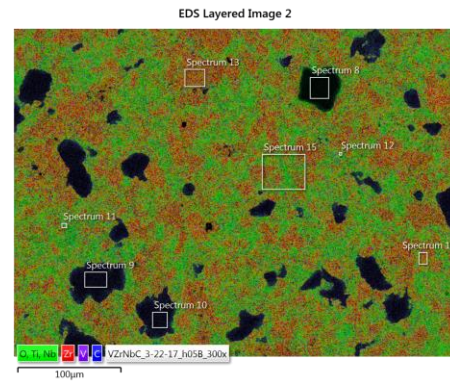


Figure 17 X-Ray Spectroscopy of Carbide Sample after Screening to 45 microns

Only recently, as of the time of this paper was written, has the micro milling equipment become operational. The authors believe using the micro mill to decrease the particle size of the carbide powders to a uniform size will result in improved material distribution.

D. Cutting Grooves

Important to the manufacturing process is the method for creating the grooves in the carbide rings as well as the center hole. Two tools are being investigated for use in this effort; a diamond wire saw and a water jet. The saw was tested on a carbide sample and successfully cut several grooves through the material. The saw has several limitations however. The saw limits the groove diameter to the width of the blade. It is difficult to work with due to the small size of the carbide rings. Also, it is not effective at cutting the center hole. The water jet is thought to be a promising candidate. Current water jet capabilities at Marshall Space Flight Center allow the groove width to be cut as small as 0.03 inches. The water jet is capable of cutting curves and can cut out the center hole. Adjusting the pressure should allow the operator to cut the grooves without cutting all the way through the ring.

Water jet tests are anticipated for the summer of 2017. Test cuts will be performed on a carbide sample. This will be followed by an attempt to produce several full size grooved fuel rings with the DCS and water jet.

V. Carbide Material Characterization

A proper understanding of the material properties of the carbides of interest is necessary to understand their performance in a reactor environment. We have reviewed previous work after reviewing available literature and have built upon past work. The authors are working to measure the thermal diffusivity of the carbide mixtures. Also, the material samples created using DCS are being tested in a hot hydrogen environment ($T > 2000\text{K}$). Hot hydrogen testing is used to verify the structural integrity and chemical stability of the produced material at relevant temperatures whilst in with the proposed hydrogen propellant.

A. Thermal Diffusivity Measurements

Thermal diffusivity measurements were attempted. Two samples were measured by heating the material with a light source to a set temperature. The material is then allowed to cool back to room temperature. The cooling rate is measured and used to determine thermal diffusivity. Multiple measurements were taken and average was found. Thermal diffusivity numbers were obtained and plotted for the two samples. For reasons unknown the samples disintegrated at relatively low temperatures. Testing in a hot hydrogen environment showed survivability at much higher temperatures, so this result is as of yet unexplained. It could possibly be the result of a preexisting fracture or other outside factor.

The data obtained is presented in Figure 13. Future work is planned to take new measurements of thermal diffusivity at much higher temperatures.

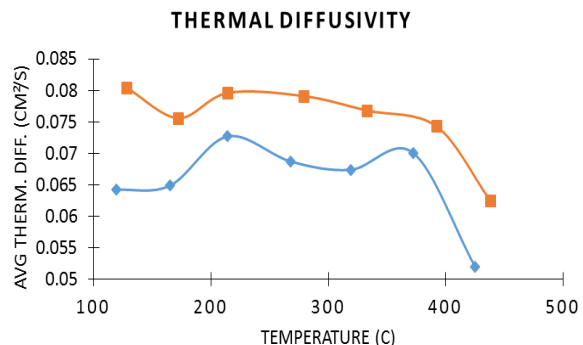


Figure 18 Thermal Diffusivity Measurements of Two Carbide Samples



Figure 19 Compact Fuel Element Environmental Test system

B. Hot Hydrogen Environment Testing

Hot hydrogen environmental testing was conducted in the Compact Fuel Element Environmental Test (CFEET) system at NASA Marshall Space Flight Center (Figure 19). CFEET has a 50 kW induction power supply and two-color pyrometers for temperature measurements up to 3000 °C. It is designed to flow hydrogen across subscale fuel materials for testing at high temperatures for up to ten hours.

An initial sample was run at a relatively low temperature to verify if the sample would fall apart similar to observed in the thermal diffusivity testing. The sample maintained structural integrity when exposed to a maximum temperature of 2000 K for 30 minutes. Subsequently, three samples were run for 30 minutes (rough timescale of a single engine burn on a Mars mission) at 2250 K. X-ray diffraction (XRD) analysis appears to show the tricarbides moving toward a solid solution. This is indicated by the shifting toward a single defined peak at an intermediate 2θ values. This XRD data can be seen in Figure 20. There does however, exist the presence of unidentified peaks post-CFEET testing. Further analysis is needed to verify if unidentified peaks are

due to the formation of free carbon, ZrC_2 , or other lower melting temperature compounds.

Overall, these results are encouraging. To date the tricarbide samples have retained their structural integrity within a hot hydrogen environment. CFEET experiments are planned to perform H_2 heat treatments at temperatures of 2500 K or greater to form solid solutions. Solid solutions refer to an ideal mixture of the tricarbides as opposed to discrete clusters of compacted binary carbide powders.

XRD and X-Ray Spectroscopy will be conducted to gain better insight of the effect of temperature on solid solution carbide formation.

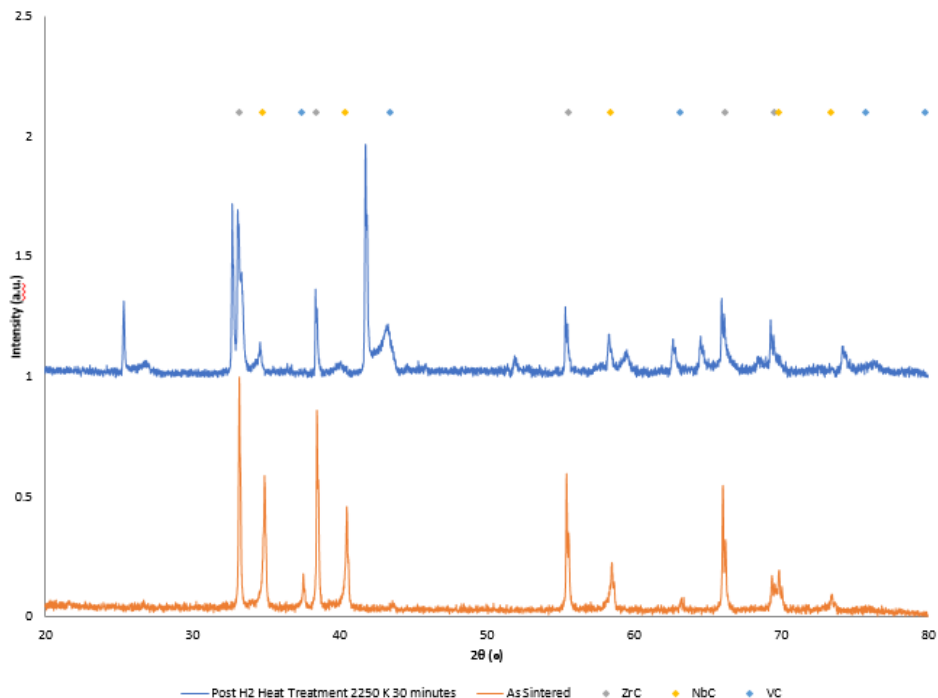


Figure 20 X-Ray Spectroscopy Analysis Before and After Testing in CFEET

VI. Conclusions

The results of the work conducted by the authors at Marshall Space Flight Center over the last several months are quite promising. Modeling has shed light on how this concept will perform in its target environment. This will aid in future design work. Fabrication experiments have come a long way in showing a viable means for manufacturing the tricarbide materials to get high density, low porosity material mixtures. Improvements in distribution are expected with powder micro milling and additional heat treatment. The team is collecting data on the thermal diffusivity of these carbides. The team is also gaining an understanding of how these tricarbides will perform in a hot hydrogen environments.

It is hopeful based on our current results that the tricarbides will be a viable fuel material. We have also shown that the new geometry of the Grooved Ring Fuel Element has promise as a new type of fuel element. We expect this will lead to nuclear thermal rocket engines with higher thrust to weight ratios, thus improving vehicle performance and allowing for more ambitious deep space exploration missions.

Acknowledgments

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